RESEARCH HIGHLIGHTS
Basic Energy Sciences Program
Geosciences Subprogram

Title: Lattice-Gas Modeling of Dispersion in Porous and Rough-Walled Fractures

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Objective: To model axial dispersion in rough-walled (alveolated) channels *via* lattice-gas automata (LGA), for both slug and step-change inlet conditions, and test the accuracy of the LGA method in a case where analytical solutions and experimental data were available for benchmarks.

Results: There was good agreement between the effective diffusion coefficient (D^*) calculated by the LGA method, and the D^* predicted by the "stagnant pocket" formalism developed by Aris, Turner, and Tsuda *et al.* The enhancement of D^* was dependent on the ratio of alveolar volume to central channel volume and the Peclet number. For $Pe \geq 5$, D^* was substantially greater than the Taylor-Aris prediction for flow between parallel flat plates. For $Pe < 3$, D^* was less than the molecular diffusion coefficient, D_m. In the absence of buoyancy, inlet conditions (pulse *vs*. step-change) had little effect on the calculated D^* ($\leq$ 3%). The effect of buoyancy, however, depends on the inlet condition; for an LGA corresponding to 1 mole % SF_6 tracer gas in air, D^* was *increased* up to 20% for the step-change, and *decreased* up to 6% for the slug.

Significance: Dispersion through fractured rocks is enhanced by surface roughness, and by diffusion in and out of the porous sidewalls. There is a similar enhancement of dispersion in the human lung, as inhaled gases diffuse into the alveoli, and in chemical engineering applications that involve porous-bed reactors. This enhancement is difficult to model by conventional numerical methods, and difficult to characterize by experiments; LGA provide a useful numerical tool for interpreting experimental data and predicting performance.

Publication: "A lattice-gas study of dispersion in alveolated channels", by Sally J. Perea-Reeves and Harlan W. Stockman, accepted in ***Chem. Eng. Sci***., 1997.